

Computer lab 4

Instructions

- Create a report to the lab solutions in PDF.
- Be concise and do not include unnecessary printouts and figures produced by the software and not required in the assignments.
- **Include all your codes as an appendix into your report.**
- A typical lab report should 2-4 pages of text plus some amount of figures plus appendix with codes.
- The lab report should be submitted via LISAM before the deadline.

Assignment 1: Computations with Metropolis-Hastings

Consider the following probability density function:

$$f(x) \propto x^5 e^{-x}, \quad x > 0$$

You can see that the distribution is known up to some constant of proportionality.

1. Use Metropolis-Hastings algorithm to generate samples from this distribution by using proposal distribution as log-normal $\text{LN}(X_t, 1)$, take some starting point. Plot the chain you obtained as a time series plot. What can you guess about the convergence of the chain? If there is a burn-in period, what can be the size of this period?
2. Perform step 1 by using chi-square distribution $\chi^2(\text{floor}(X_t + 1))$ as proposal distribution where $\text{floor}(x)$ means integer part of x .
3. Compare the results of steps 1 and 2 and make conclusions.
4. Generate 10 MCMC sequences using the generator from the step 2 and with starting points 1, 2, ..., or 10. Use Gelman-Rubin method to analyze convergence of these sequences.
5. Estimate $\int_0^\infty x \cdot f(x) dx$ using the samples from steps 1 and 2.
6. The distribution generated is in fact a gamma distribution. Look in the literature and define the actual value of the integral. Compare it with the one you obtained.

Assignment 2: Gibbs sampling

A concentration of a certain chemical was measured in a water sample, and the result was stored in the data **chemical.RData** having the following variables:

- X: day of the measurement
- Y: measured concentration of the chemical.

The instrument used to measure the concentration had certain accuracy; this is why the measurements can be treated as noisy. Your purpose is to restore the expected concentration values.

1. Import the data to R and plot the dependence of Y on X. What kind of model is reasonable to use here?
2. A researcher has decided to use the following (random-walk) Bayesian model (n =number of observations, $\boldsymbol{\mu} = (\mu_1, \dots, \mu_n)$ are unknown parameters):

$$Y_i \sim N(\mu_i, \text{var} = 0.2), i = 1, \dots, n$$

where the prior is

$$p(\mu_1) = 1$$

$$p(\mu_{i+1} | \mu_i) = N(\mu_i, 0.2), i = 1, \dots, n - 1$$

Present the formulas showing the likelihood $p(\mathbf{Y} | \boldsymbol{\mu})$ and the prior $p(\boldsymbol{\mu})$ (hint: a chain rule can be used here $p(\boldsymbol{\mu}) = p(\mu_1)p(\mu_2 | \mu_1)p(\mu_3 | \mu_2) \dots p(\mu_n | \mu_{n-1})$)

3. Use the Bayes theorem to get the posterior up to a constant of proportionality, and then find out the distributions for $\mu_i | \boldsymbol{\mu}_{-i}, \mathbf{Y}$ where $\boldsymbol{\mu}_{-i}$ is a vector containing all μ values except of μ_i
 - a. Hint A: consider separate formulas for $\mu_1 | \mu_{-1}, \mathbf{Y}$, $\mu_{50} | \mu_{-50}, \mathbf{Y}$ and then a formula for all remaining $\mu_i | \boldsymbol{\mu}_{-i}, \mathbf{Y}$
 - b. Hint B: $\exp\left(-\frac{1}{d}((x-a)^2 + (x-b)^2)\right) \propto \exp\left(-\frac{\left(x - \frac{a+b}{2}\right)^2}{d/2}\right)$
 - c. Hint C: $\exp\left(-\frac{1}{d}((x-a)^2 + (x-b)^2 + (x-c)^2)\right) \propto \exp\left(-\frac{\left(x - \frac{a+b+c}{3}\right)^2}{d/3}\right)$
4. Use the distributions derived in step 3 to implement a Gibbs sampler that uses $\boldsymbol{\mu}^0 = (0, \dots, 0)$ as a starting point. Run the Gibbs sampler to obtain 1000 values of $\boldsymbol{\mu}$ and then compute the expected value of $\boldsymbol{\mu}$ by using Monte Carlo approach. Plot the expected value of $\boldsymbol{\mu}$ versus X and Y versus X in the same graph. Does it seem that you have managed to remove the noise? Does it seem that the expected value of $\boldsymbol{\mu}$ can catch the true underlying dependence between Y and X?
5. Make a trace plot for μ_{50} and comment on the burn-in period and convergence.

Submission procedure

Assume that X is the current lab number.

If you are neither speaker nor opponent for this lab,

- Submit your report using *Lab X* item in the *Submissions* folder before the deadline.
- Make sure that you or some of your group members submits the group report using *Lab X group report* in the *Submissions* folder before the deadline

If you are a speaker for this lab,

- Submit your report using *Lab X* item in the *Submissions* folder before the deadline.
- Make sure that you or some of your group members does the following before the deadline:
 - submits the group report using *Lab X group report* in the *Submissions* folder before the deadline
 - Goes to Study room *Speakers X* → *Documents* and opens file *Password X.txt*. Then the student should put your group report into ZIP file *Lab X.zip* and protect it with a password you found in *Password X.txt*
 - Uploads the file to *Collaborative workspace* folder

If you are opponent for this lab,

- Submit your report using *Lab X* item in the *Submissions* folder before the deadline.
- Make sure that you or some of your group members submits the group report using *Lab X group report* in the *Submissions* folder before the deadline
- After the deadline for the lab has passed, go to Collaborative workspace folder and download *Lab X.zip*. Open the PDF in this ZIP file by using the password available in *Course Documents* → *Password X.txt*, read it carefully and **prepare at least two questions/comments/improvement suggestions** in order to put them at the seminar (i.e. at least two questions per opponent)